

THE SQUARE AND CUBE OF THE TRANSITION MATRIX OF THE DISCRETE-TIME QUANTUM WALK ON A GRAPH

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Abstract. We give a new proof of a determinant expression for the second weighted zeta function of a graph by using the method of Watanabe and Fukumizu [23]. Also, we give another proof of a result by Emms et al. [3] on spectra of the positive support of the square of the transition matrix of the discrete-time quantum walk on a graph. Furthermore, we determine the structure of the positive support of the cube of the transition matrix under a certain condition.

1 Introduction

As a quantum counterpart of the classical random walk, the quantum walk has recently attracted much attention for various fields. The review and book on quantum walks are Ambainis [1], Kempe [10], Kendon [11], Konno [12], Venegas-Andraca [22], for examples. Quantum walks of graphs were applied in graph isomorphism problems. Graph isomorphism problems determine whether two graphs are isomorphic. Shiau et al. [18] first pointed out the deficiency of the simplest classical algorithm and continuous-time one particle quantum random walks in distinguishing some non-isomorphic graphs. Emms et al. [4] introduced a graph-spectral technique induced by discrete-time quantum walks to distinguish two non-isomorphic graphs that are cospectral with respect to standard matrix representations. Gambel et al. [6] developed a method of characterizing the additional power that quantum

Abbr. title: The transition matrix of a quantum walk on a graph

AMS 2000 subject classifications: 60F05, 05C50, 15A15, 05C60

PACS: 03.67.Lx, 05.40.Fb, 02.50.Cw

Keywords: Quantum walk, transition matrix, Ihara zeta function

walks of interacting particles have for distinguishing non-isomorphic regular graphs. Emms et al. [3] treated spectra of the transition matrix and its positive support of the discrete-time quantum walk on a graph, and showed that the third power of the transition matrix outperforms the graph spectra methods in distinguishing strongly regular graphs. Godsil and Guo [7] gave new proofs of the results of Emms et al. [3].

Already, the Ihara zeta function of a graph obtained various success related to graph spectra. Ihara zeta functions of graphs started from Ihara zeta functions of regular graphs by Ihara [9]. Originally, Ihara [9] presented p -adic Selberg zeta functions of discrete groups, and showed that its reciprocal is an explicit polynomial. Serre [17] pointed out that the Ihara zeta function is the zeta function of the quotient T/Γ (a finite regular graph) of the one-dimensional Bruhat-Tits building T (an infinite regular tree) associated with $GL(2, k_p)$. A zeta function of a regular graph G associated with a unitary representation of the fundamental group of G was developed by Sunada [20, 21]. Hashimoto [8] treated multivariable zeta functions of bipartite graphs. Bass [2] generalized Ihara's result on the zeta function of a regular graph to an irregular graph, and showed that its reciprocal is again a polynomial. Various proofs of Bass' Theorem were given by Stark and Terras [19], Foata and Zeilberger [5], Kotani and Sunada [14]. Sato [16] defined a new zeta function of a graph by using not an infinite product but a determinant.

Ren et al. [15] found an interesting relationship between the Ihara zeta function and the discrete-time quantum walk on a graph, and showed that the support of the transition matrix of the discrete-time quantum walk is equal to the Perron-Frobenius operator (the edge matrix) related to the Ihara zeta function. Based on this analysis, Ren et al. explained that the Ihara zeta function can not distinguish cospectral regular graphs.

The rest of the paper is organized as follows. Section 2 gives the definition of the transition matrix of the discrete-time quantum walk on a graph, and review results on it. In Sect. 3, we define the Ihara zeta function and the second weighted zeta function of a graph, and present their determinant expressions. In Sect. 4, we state a short review on the characteristic polynomials and the spectra of the transition matrix and its positive support. In Sect. 5, we give a new proof of Theorem 3.2 by using the method of Watanabe and Fukumizu [23]. In Sect. 7, we give another proof of a result by Emms et al. [3] on spectra of the positive support of the square of the transition matrix. In Sect. 8, we treat the positive support of the cube of the transition matrix.

2 Definition of the transition matrix of a quantum walk on a graph

Graphs treated here are finite. Let $G = (V(G), E(G))$ be a connected graph (possibly multiple edges and loops) with the set $V(G)$ of vertices and the set $E(G)$ of unoriented edges uv joining two vertices u and v . For $uv \in E(G)$, an arc (u, v) is the oriented edge from u to v . Set $D(G) = \{(u, v), (v, u) | uv \in E(G)\}$. For $e = (u, v) \in D(G)$, set $u = o(e)$ and $v = t(e)$. Furthermore, let $e^{-1} = (v, u)$ be the *inverse* of $e = (u, v)$. The *degree* $\deg v = \deg_G v$ of a vertex v of G is the number of edges incident to v . For a natural number k , a graph G is called *k -regular* if $\deg_G v = k$ for each vertex v of G .

A discrete-time quantum walk is a quantum analog of the classical random walk on

a graph whose state vector is governed by a matrix called the transition matrix. Let G be a connected graph with n vertices and m edges, $V(G) = \{v_1, \dots, v_n\}$ and $D(G) = \{e_1, \dots, e_m, e_1^{-1}, \dots, e_m^{-1}\}$. Set $d_j = d_{u_j} = \deg v_j$ for $i = 1, \dots, n$. The *transition matrix* $\mathbf{U} = \mathbf{U}(G) = (U_{ef})_{e,f \in D(G)}$ of G is defined by

$$U_{ef} = \begin{cases} 2/d_{t(f)} (= 2/d_{o(e)}) & \text{if } t(f) = o(e) \text{ and } f \neq e^{-1}, \\ 2/d_{t(f)} - 1 & \text{if } f = e^{-1}, \\ 0 & \text{otherwise.} \end{cases}$$

We introduce the *positive support* $\mathbf{F}^+ = (F_{ij}^+)$ of a real matrix $\mathbf{F} = (F_{ij})$ as follows:

$$F_{ij}^+ = \begin{cases} 1 & \text{if } F_{ij} > 0, \\ 0 & \text{otherwise.} \end{cases}$$

Let G be a connected graph. If the degree of each vertex of G is not less than 2, i.e., $\delta(G) \geq 2$, then G is called an *md2 graph*.

The transition matrix of a discrete-time quantum walk in a graph is closely related to the Ihara zeta function of a graph. We state a relationship between the discrete-time quantum walk and the Ihara zeta function of a graph by Ren et al. [15].

THEOREM 2.1 (REN, ALEKSIC, EMMS, WILSON AND HANCOCK [15]) *Let $\mathbf{B} - \mathbf{J}_0$ be the Perron-Frobenius operator (or the edge matrix) of a simple graph subject to the md2 constraint, where the edge matrix is defined in Section 3. Let \mathbf{U} be the transition matrix of the discrete-time quantum walk on G . Then the $\mathbf{B} - \mathbf{J}_0$ is the positive support of the transpose of \mathbf{U} , i.e.,*

$$\mathbf{B} - \mathbf{J}_0 = ({}^T\mathbf{U})^+,$$

where ${}^T\mathbf{U}$ is the transpose of \mathbf{U} .

3 The Ihara zeta function of a graph

Let G be a connected graph. Then a *path* P of length n in G is a sequence $P = (e_1, \dots, e_n)$ of n arcs such that $e_i \in D(G)$, $t(e_i) = o(e_{i+1})$ ($1 \leq i \leq n-1$), where indices are treated *mod* n . If $o(e_i) = v_{i-1}$ and $t(e_i) = v_i$ for $i = 1, \dots, n$, then we write $C = (v_0, e_1, v_1, \dots, v_{n-1}, e_n, v_n)$. Set $|P| = n$, $o(P) = o(e_1)$ and $t(P) = t(e_n)$. Also, P is called an $(o(P), t(P))$ -*path*. Furthermore, P is called an (e_1, e_n) -*path*. We say that a path $P = (e_1, \dots, e_n)$ has a *backtracking* if $e_{i+1}^{-1} = e_i$ for some i ($1 \leq i \leq n-1$). A (v, w) -path is called a *v-cycle* (or *v-closed path*) if $v = w$. The *inverse cycle* of a cycle $C = (e_1, \dots, e_n)$ is the cycle $C^{-1} = (e_n^{-1}, \dots, e_1^{-1})$.

We introduce an equivalence relation between cycles. Two cycles $C_1 = (e_1, \dots, e_m)$ and $C_2 = (f_1, \dots, f_m)$ are called *equivalent* if there exists k such that $f_j = e_{j+k}$ for all j . The inverse cycle of C is in general not equivalent to C . Let $[C]$ be the equivalence class which contains a cycle C . Let B^r be the cycle obtained by going r times around a cycle B . Such a cycle is called a *power* of B . A cycle C is *reduced* if C has no backtracking. Furthermore, a cycle C is *prime* if it is not a power of a strictly smaller cycle. Note that each equivalence class of prime, reduced cycles of a graph G corresponds to a unique conjugacy class of the fundamental group $\pi_1(G, v)$ of G at a vertex v of G .

A cycle $C = (v_0, e_1, v_1, \dots, v_{n-1}, e_n, v_n)$ ($v_0 = v_n$) is called *essential* if all vertices of C except v_0, v_n are distinct. An essential cycle is the same as a dicycle in standard books on graph theory. Note that any essential cycle is a prime, reduced cycle, and any prime, reduced cycle is a union of disjoint essential cycles. The *girth* $g(G)$ of a graph G is the minimum length of essential cycles in G .

The *Ihara zeta function* of a graph G is a function of $t \in \mathbf{C}$ with $|t|$ sufficiently small, defined by

$$\mathbf{Z}(G, t) = \mathbf{Z}_G(t) = \prod_{[C]} (1 - t^{|C|})^{-1},$$

where $[C]$ runs over all equivalence classes of prime, reduced cycles of G .

Let G be a connected graph with n vertices and m edges. Two $2m \times 2m$ matrices $\mathbf{B} = \mathbf{B}(G) = (\mathbf{B}_{ef})_{e,f \in D(G)}$ and $\mathbf{J}_0 = \mathbf{J}_0(G) = (\mathbf{J}_{ef})_{e,f \in D(G)}$ are defined as follows:

$$\mathbf{B}_{ef} = \begin{cases} 1 & \text{if } t(e) = o(f), \\ 0 & \text{otherwise,} \end{cases} \quad \mathbf{J}_{ef} = \begin{cases} 1 & \text{if } f = e^{-1}, \\ 0 & \text{otherwise.} \end{cases}$$

Then the matrix $\mathbf{B} - \mathbf{J}_0$ is called the *edge matrix* of G .

THEOREM 3.1 (HASHIMOTO [8]; BASS [2]) *Let G be a connected graph. Then the reciprocal of the Ihara zeta function of G is given by*

$$\mathbf{Z}(G, t)^{-1} = \det(\mathbf{I}_{2m} - t(\mathbf{B} - \mathbf{J}_0)) = (1 - t^2)^{r-1} \det(\mathbf{I}_n - t\mathbf{A}(G) + t^2(\mathbf{D} - \mathbf{I}_n)),$$

where \mathbf{I}_n is the $n \times n$ identity matrix, r and $\mathbf{A}(G)$ are the Betti number and the adjacency matrix of G , respectively, and $\mathbf{D} = (d_{ii})$ is the diagonal matrix with $d_{ii} = \deg v_i$, $V(G) = \{v_1, \dots, v_n\}$.

Let G be a connected graph and $V(G) = \{v_1, \dots, v_n\}$. Then we consider an $n \times n$ matrix $\mathbf{W} = (w_{ij})_{1 \leq i, j \leq n}$ with ij entry nonzero complex number w_{ij} if $(v_i, v_j) \in D(G)$, and $w_{ij} = 0$ otherwise. The matrix $\mathbf{W} = \mathbf{W}(G)$ is called the *weighted matrix* of G . Furthermore, let $w(v_i, v_j) = w_{ij}$, $v_i, v_j \in V(G)$ and $w(e) = w_{ij}$, $e = (v_i, v_j) \in D(G)$. For each path $P = (e_1, \dots, e_r)$ of G , the *norm* $w(P)$ of P is defined as follows: $w(P) = w(e_1)w(e_2) \cdots w(e_r)$.

Let G be a connected graph with n vertices and m edges, and $\mathbf{W} = \mathbf{W}(G)$ a weighted matrix of G . A $2m \times 2m$ matrix $\mathbf{B}_w = \mathbf{B}_w(G) = (\mathbf{B}_{ef}^{(w)})_{e,f \in D(G)}$ is defined as follows:

$$\mathbf{B}_{ef}^{(w)} = \begin{cases} w(f) & \text{if } t(e) = o(f), \\ 0 & \text{otherwise.} \end{cases}$$

Then the *second weighted zeta function* of G is defined by

$$\mathbf{Z}_1(G, w, t) = \det(\mathbf{I}_{2m} - t(\mathbf{B}_w - \mathbf{J}_0))^{-1}.$$

If $w(e) = 1$ for any $e \in D(G)$, then the second weighted zeta function of G is the Ihara zeta function of G .

THEOREM 3.2 (SATO [16]) *Let G be a connected graph, and let $\mathbf{W} = \mathbf{W}(G)$ be a weighted matrix of G . Then the reciprocal of the second weighted zeta function of G is given by*

$$\mathbf{Z}_1(G, w, t)^{-1} = (1 - t^2)^{m-n} \det(\mathbf{I}_n - t\mathbf{W}(G) + t^2(\mathbf{D}_w - \mathbf{I}_n)),$$

where $n = |V(G)|$, $m = |E(G)|$ and $\mathbf{D}_w = (d_{ij})$ is the diagonal matrix with $d_{ii} = \sum_{o(e)=v_i} w(e)$, $V(G) = \{v_1, \dots, v_n\}$.

Stark and Terras [19] defined the edge zeta function of a graph G with n vertices. Let G be a connected graph and $D(G) = \{e_1, \dots, e_m, e_{m+1}, \dots, e_{2m}\} (e_{m+i} = e_i^{-1} (1 \leq i \leq m))$. We introduce $2m$ variables u_1, \dots, u_{2m} , and set $g(C) = u_{i_1} \cdots u_{i_k}$ for each cycle $C = (e_{i_1}, \dots, e_{i_k})$ of G . Then the *edge zeta function* $\zeta_G(u)$ of G is defined by

$$\zeta_G(\mathbf{u}) = \prod_{[C]} (1 - g(C))^{-1},$$

where $[C]$ runs over all equivalence classes of prime, reduced cycles of G .

THEOREM 3.3 (STARK AND TERRAS [19]) *Let G be a connected graph with m edges. Then*

$$\zeta_G(\mathbf{u})^{-1} = \det(\mathbf{I}_{2m} - (\mathbf{B} - \mathbf{J}_0)\mathbf{U}) = \det(\mathbf{I}_{2m} - \mathbf{U}(\mathbf{B} - \mathbf{J}_0)),$$

where

$$\mathbf{U} = \text{diag}(u_1, \dots, u_m, u_{m+1}, \dots, u_{2m}).$$

Watanabe and Fukumizu [23] presented a determinant expression for the edge zeta function of a graph G with n vertices by $n \times n$ matrices. Then we define an $n \times n$ matrix $\widehat{\mathbf{A}} = \widehat{\mathbf{A}}(G) = (a_{xy})$ as follows:

$$a_{xy} = \begin{cases} u_{(x,y)} / (1 - u_{(x,y)} u_{(y,x)}) & \text{if } (x, y) \in D(G), \\ 0 & \text{otherwise.} \end{cases}$$

Furthermore, an $n \times n$ matrix $\widehat{\mathbf{D}} = \widehat{\mathbf{D}}(G) = (d_{xy})$ is the diagonal matrix defined by

$$d_{xx} = \sum_{o(e)=x} \frac{u_e u_{e^{-1}}}{1 - u_e u_{e^{-1}}}.$$

THEOREM 3.4 (WATANABE AND FUKUMIZU [23])

$$\zeta_G(\mathbf{u})^{-1} = \det(\mathbf{I}_n + \widehat{\mathbf{D}} - \widehat{\mathbf{A}}) \prod_{i=1}^m (1 - u_{e_i} u_{e_i^{-1}}).$$

4 The characteristic polynomial of the transition matrix

We present a formula for the characteristic polynomial of \mathbf{U} . Let G be a connected graph with n vertices and m edges. Then the $n \times n$ matrix $\mathbf{T}(G) = (T_{uv})_{u,v \in V(G)}$ is given as follows:

$$T_{uv} = \begin{cases} 1/(\deg_G u) & \text{if } (u, v) \in D(G), \\ 0 & \text{otherwise.} \end{cases}$$

THEOREM 4.1 (KONNNO AND SATO [13]) *Let G be a connected graph with n vertices v_1, \dots, v_n and m edges. Then, for the transition matrix \mathbf{U} of G , we have*

$$\begin{aligned} \det(\lambda \mathbf{I}_{2m} - \mathbf{U}) &= (\lambda^2 - 1)^{m-n} \det((\lambda^2 + 1)\mathbf{I}_n - 2\lambda \mathbf{T}(G)) \\ &= \frac{(\lambda^2 - 1)^{m-n} \det((\lambda^2 + 1)\mathbf{D} - 2\lambda \mathbf{A}(G))}{d_{v_1} \cdots d_{v_n}}. \end{aligned}$$

We can express the spectra of the transition matrix \mathbf{U} by means of those of $\mathbf{T}(G)$ (see [3]). Let $\text{Spec}(\mathbf{F})$ be the spectra of a square matrix \mathbf{F} .

COROLLARY 4.2 (EMMS, HANCOCK, SEVERINI AND WILSON [3]) *Let G be a connected graph with n vertices and m edges. The transition matrix \mathbf{U} has $2n$ eigenvalues of the form*

$$\lambda = \lambda_T \pm i\sqrt{1 - \lambda_T^2},$$

where λ_T is an eigenvalue of the matrix $\mathbf{T}(G)$. The remaining $2(m - n)$ eigenvalues of \mathbf{U} are ± 1 with equal multiplicities.

Emms et al. [3] determined the spectra of the transition matrix \mathbf{U} by examining the elements of the transition matrix of a graph and using the properties of the eigenvector of a matrix. And now, we could explicitly obtain the spectra of the transition matrix \mathbf{U} from its characteristic polynomial.

Next, we state about the positive support of the transition matrix of a graph.

By Theorem 2.1, Emms et al. [3] expressed the spectra of the positive support \mathbf{U}^+ of the transition matrix of a regular graph G by means of those of the adjacency matrix $\mathbf{A}(G)$ of G .

THEOREM 4.3 (EMMS, HANCOCK, SEVERINI AND WILSON [3]) *Let G be a connected k -regular graph with n vertices and m edges, and $k \geq 2$. The positive support \mathbf{U}^+ has $2n$ eigenvalues of the form*

$$\lambda = \frac{\lambda_A}{2} \pm i\sqrt{k - 1 - \lambda_A^2/4},$$

where λ_A is an eigenvalue of the matrix $\mathbf{A}(G)$. The remaining $2(m - n)$ eigenvalues of \mathbf{U}^+ are ± 1 with equal multiplicities.

Godsil and Guo [7] presented a new proof of Theorem 4.3 by using linear algebraic technique.

Konnno and Sato [13] gave the following formula of the characteristic polynomial of \mathbf{U}^+ , and obtained a simple proof of Theorem 4.3.

PROPOSITION 4.4 (KONNNO AND SATO [13])

$$\det(\lambda \mathbf{I}_{2m} - \mathbf{U}^+) = (\lambda^2 - 1)^{m-n} \det((\lambda^2 - 1)\mathbf{I}_n - \lambda \mathbf{A}(G) + \mathbf{D}).$$

5 Another proof of Theorem 3.2

We present another proof of Theorem 3.2 by using the method of Watanabe and Fukumizu [23].

THEOREM 5.1 *Let G be a connected graph with n vertices and m edges, and let $\mathbf{W} = \mathbf{W}(G)$ be a weighted matrix of G . Then the reciprocal of the second weighted zeta function of G is given by*

$$\mathbf{Z}_1(G, w, t)^{-1} = (1 - t^2)^{m-n} \det(\mathbf{I}_n - t\mathbf{W}(G) + t^2(\mathbf{D}_w - \mathbf{I}_n)),$$

where $n = |V(G)|$, $m = |E(G)|$ and $\mathbf{D}_w = (d_{ij})$ is the diagonal matrix with $d_{ii} = \sum_{o(e)=v_i} w(e)$, $V(G) = \{v_1, \dots, v_n\}$.

Proof . Let $D(G) = \{f_1, \dots, f_m, f_1^{-1}, \dots, f_m^{-1}\}$. Arrange arcs of G as follows:

$$f_1, f_1^{-1}, \dots, f_m, f_m^{-1}.$$

By the definition of the second weighted zeta function of G , we have

$$\mathbf{Z}_1(G, w, t)^{-1} = \det(\mathbf{I}_{2m} - t(\mathbf{B}_w - \mathbf{J}_0)).$$

Now, let $\mathbf{K} = (\mathbf{K}_{ev})_{e \in D(G); v \in V(G)}$ be the $2m \times n$ matrix defined as follows:

$$\mathbf{K}_{ev} := \begin{cases} w(e) & \text{if } o(e) = v, \\ 0 & \text{otherwise.} \end{cases}$$

Furthermore, we define the $2m \times n$ matrix $\mathbf{L} = (\mathbf{L}_{ev})_{e \in D(G); v \in V(G)}$ as follows:

$$\mathbf{L}_{ev} := \begin{cases} 1 & \text{if } t(e) = v, \\ 0 & \text{otherwise.} \end{cases}$$

Then we have

$$\mathbf{L}^T \mathbf{K} = \mathbf{B}_w.$$

Thus,

$$\begin{aligned} \det(\mathbf{I}_{2m} + t\mathbf{J}_0 - t\mathbf{B}_w) &= \det(\mathbf{I}_{2m} + t\mathbf{J}_0 - t\mathbf{L}^T \mathbf{K}) \\ &= \det(\mathbf{I}_{2m} - t\mathbf{L}^T \mathbf{K}(\mathbf{I}_{2m} + t\mathbf{J}_0)^{-1}) \det(\mathbf{I}_{2m} + t\mathbf{J}_0). \end{aligned}$$

But, if \mathbf{A} and \mathbf{B} are a $m \times n$ and $n \times m$ matrices, respectively, then we have

$$\det(\mathbf{I}_m - \mathbf{A}\mathbf{B}) = \det(\mathbf{I}_n - \mathbf{B}\mathbf{A}).$$

Thus, we have

$$\det(\mathbf{I}_{2m} + t\mathbf{J}_0 - t\mathbf{B}_w) = \det(\mathbf{I}_n - t^T \mathbf{K}(\mathbf{I}_{2m} + t\mathbf{J}_0)^{-1} \mathbf{L}) \det(\mathbf{I}_{2m} + t\mathbf{J}_0).$$

Next, we have

$$\det(\mathbf{I}_{2m} + t\mathbf{J}_0) = (1 - t^2)^m.$$

Furthermore, we have

$$(\mathbf{I}_{2m} + t\mathbf{J})^{-1} = \mathbf{I}_m \otimes \begin{bmatrix} 1/(1-t^2) & -t/(1-t^2) \\ -t/(1-t^2) & 1/(1-t^2) \end{bmatrix}.$$

But, for an arc $(x, y) \in D(G)$,

$$({}^T\mathbf{K}(\mathbf{I}_{2m} + t\mathbf{J}_0)^{-1}\mathbf{L})_{xy} = w(x, y)/(1-t^2).$$

In the case of $x = y$,

$$({}^T\mathbf{K}(\mathbf{I}_{2m} + t\mathbf{J}_0)^{-1}\mathbf{L})_{xx} = - \sum_{o(e)=x} \frac{tw(e)}{1-t^2}.$$

Thus,

$$\det(\mathbf{I}_n - t {}^T\mathbf{K}(\mathbf{I}_{2m} + t\mathbf{J}_0)^{-1}\mathbf{L}) = \det(\mathbf{I}_n + \frac{t^2}{1-t^2}\mathbf{D}_w - \frac{t}{1-t^2}\mathbf{W}(G)).$$

Therefore, it follows that

$$\begin{aligned} \mathbf{Z}_1(G, w, t)^{-1} &= (1-t^2)^m \cdot \frac{1}{(1-t^2)^n} \det((1-t^2)\mathbf{I}_n - t\mathbf{W}(G) + t^2\mathbf{D}_w) \\ &= (1-t^2)^{m-n} \det(\mathbf{I}_n - t\mathbf{W}(G) + t^2(\mathbf{D}_w - \mathbf{I}_n)). \end{aligned}$$

□

6 The positive support of the square of the transition matrix of a graph

By Proposition 4.4, we express the spectra of the positive support \mathbf{U}^+ of the square of the transition matrix of a regular graph G by means of those of the adjacency matrix $\mathbf{A}(G)$ of G (see [3]).

Emms et al. [3] found the eigenvalues of the positive support $(\mathbf{U}^2)^+$ of the second power \mathbf{U}^2 of the transition matrix \mathbf{U} of a regular graph (c.f., [7]). Furthermore, Godsil and Guo [7] expressed $(\mathbf{U}^2)^+$ in terms of \mathbf{U}^+ by using linear algebraic technique, and presented another proof of the result of Emms et al. [3].

We directly present the spectrum of $(\mathbf{U}^2)^+$ from the characteristic polynomial of $(\mathbf{U}^2)^+$ by using Proposition 4.4.

THEOREM 6.1 (EMMS, HANCOCK, SEVERINI AND WILSON [3]) *Let G be a connected k -regular graph with n vertices and m edges. Suppose that $k > 2$. The positive support $(\mathbf{U}^2)^+$ has $2n$ eigenvalues of the form*

$$\lambda = \frac{\lambda_A^2 - 2k + 4}{2} \pm i \frac{\lambda_A \sqrt{4k - 4 - \lambda_A^2}}{2},$$

where λ_A is an eigenvalue of the matrix $\mathbf{A}(G)$. The remaining $2(m-n)$ eigenvalues of \mathbf{U}^+ are 2.

Proof. Let G be a connected graph with n vertices and m edges, $V(G) = \{v_1, \dots, v_n\}$ and $D(G) = \{e_1, \dots, e_m, e_1^{-1}, \dots, e_m^{-1}\}$. Since G is k -regular, we have $\mathbf{D} = k\mathbf{I}_n$. Since $k > 2$, by Theorem 4.1 of Godsil and Guo [7], we have

$$(\mathbf{U}^2)^+ = (\mathbf{U}^+)^2 + \mathbf{I}_{2m}.$$

Thus, by Proposition 4.4,

$$\begin{aligned} \det(\mathbf{I}_{2m} - t(\mathbf{U}^2)^+) &= \det(\mathbf{I}_{2m} - t((\mathbf{U}^+)^2 + \mathbf{I}_{2m})) = \det((1-t)\mathbf{I}_{2m} - t(\mathbf{U}^+)^2) \\ &= (1-t)^{2m} \det(\mathbf{I}_{2m} - \frac{t}{1-t}(\mathbf{U}^+)^2) \\ &= (1-t)^{2m} \det(\mathbf{I}_{2m} - \sqrt{\frac{t}{1-t}}\mathbf{U}^+) \det(\mathbf{I}_{2m} + \sqrt{\frac{t}{1-t}}\mathbf{U}^+) \\ &= (1-t)^{2m} (\frac{t}{1-t})^{2m} \det(\sqrt{\frac{1-t}{t}}\mathbf{I}_{2m} - \mathbf{U}^+) \det(\sqrt{\frac{1-t}{t}}\mathbf{I}_{2m} + \mathbf{U}^+) \\ &= t^{2m} (\frac{1-t}{t} - 1)^{m-n} \det((\frac{1-t}{t} - 1)\mathbf{I}_n - \sqrt{\frac{1-t}{t}}\mathbf{A}(G) + k\mathbf{I}_n) \\ &\times (\frac{1-t}{t} - 1)^{m-n} \det((\frac{1-t}{t} - 1)\mathbf{I}_n + \sqrt{\frac{1-t}{t}}\mathbf{A}(G) + k\mathbf{I}_n) \\ &= t^{2n} (1-2t)^{2m-2n} \det(\frac{kt-2t+1}{t}\mathbf{I}_n - \sqrt{\frac{1-t}{t}}\mathbf{A}(G)) \det(\frac{kt-2t+1}{t}\mathbf{I}_n + \sqrt{\frac{1-t}{t}}\mathbf{A}(G)) \\ &= (1-2t)^{2m-2n} \det((kt-2t+1)\mathbf{I}_n - \sqrt{t(1-t)}\mathbf{A}(G)) \det((kt-2t+1)\mathbf{I}_n + \sqrt{t(1-t)}\mathbf{A}(G)). \end{aligned}$$

Set $t = 1/\lambda$. Then we have

$$\begin{aligned} \det(\mathbf{I}_{2m} - 1/\lambda(\mathbf{U}^2)^+) &= (1-2/\lambda)^{2m-2n} \det\left(\left(\frac{k-2}{\lambda} + 1\right)\mathbf{I}_n - \sqrt{\frac{1}{\lambda}(1-\frac{1}{\lambda})}\mathbf{A}(G)\right) \\ &\times \det\left(\left(\frac{k-2}{\lambda} + 1\right)\mathbf{I}_n + \sqrt{\frac{1}{\lambda}(1-\frac{1}{\lambda})}\mathbf{A}(G)\right) \\ &= (1-2/\lambda)^{2m-2n} \prod_{\lambda_A \in \text{Spec}(\mathbf{A}(G))} \left(\left(\frac{k-2}{\lambda} + 1\right)^2 - \frac{\lambda-1}{\lambda^2}\lambda_A^2\right). \end{aligned}$$

Therefore, it follows that

$$\begin{aligned} \det(\lambda\mathbf{I}_{2m} - (\mathbf{U}^2)^+) &= (\lambda-2)^{2m-2n} \prod_{\lambda_A \in \text{Spec}(\mathbf{A}(G))} ((k-2+\lambda)^2 - (\lambda-1)\lambda_A^2) \\ &= (\lambda-2)^{2m-2n} \prod_{\lambda_A \in \text{Spec}(\mathbf{A}(G))} (\lambda^2 + (2k-4-\lambda_A^2)\lambda + (k-2)^2 + \lambda_A^2). \end{aligned}$$

Solving $\lambda^2 + (2k-4-\lambda_A^2)\lambda + (k-2)^2 + \lambda_A^2 = 0$, we get

$$\lambda = \frac{\lambda_A^2 - 2k + 4}{2} \pm i \frac{\lambda_A \sqrt{4k-4-\lambda_A^2}}{2}.$$

The result follows. \square

7 The positive support of the cube of the transition matrix of a graph

We proceed arguments along Godsil and Guo [7].

Let G be a connected graph with n vertices and m edges. Then we define two $n \times 2m$ matrices \mathbf{D}_h and \mathbf{D}_t of G as follows:

$$(\mathbf{D}_h)_{ve} = \begin{cases} 1 & \text{if } t(e) = v, \\ 0 & \text{otherwise,} \end{cases} \quad (\mathbf{D}_t)_{ve} = \begin{cases} 1 & \text{if } o(e) = v, \\ 0 & \text{otherwise,} \end{cases}$$

For two matrices \mathbf{D}_h and \mathbf{D}_t , the following results holds.

PROPOSITION 7.1 (GODSIL AND GUO [7]) 1. :

$$\mathbf{D}_h^T \mathbf{D}_t = {}^T \mathbf{A}(G) \text{ and } {}^T \mathbf{D}_t \mathbf{D}_h = {}^T \mathbf{B}.$$

2. : If G is k -regular, then

$$\mathbf{U} = \frac{2}{k} {}^T \mathbf{D}_t \mathbf{D}_h - \mathbf{J}_0.$$

3. :

$$\mathbf{J}_0^T \mathbf{D}_h = {}^T \mathbf{D}_t \text{ and } \mathbf{J}_0^T \mathbf{D}_t = {}^T \mathbf{D}_h.$$

Now, let G be a connected k -regular graph with $k > 2$ and $g(G) > 4$. Then we consider the structure of the positive support $(\mathbf{U}^3)^+$ of the cube of the transition matrix \mathbf{U} . Since all nonzero elements of \mathbf{B} and ${}^T \mathbf{U}$ are in the same place, we treat \mathbf{B}^3 and ${}^T \mathbf{U}^3$ in parallel.

Let $\mathbf{T} = \mathbf{B} - \mathbf{J}_0$ and $\mathbf{P} = \mathbf{J}_0$. Then we have

$$\mathbf{B} = \mathbf{T} + \mathbf{P} \text{ and } {}^T \mathbf{U}^+ = \mathbf{B} - \mathbf{P}.$$

Thus, we have

$$\mathbf{B}^3 = (\mathbf{T} + \mathbf{P})^3 = \mathbf{T}^3 + \mathbf{T}^2 \mathbf{P} + \mathbf{TPT} + \mathbf{TP}^2 + \mathbf{PT}^2 + \mathbf{PTP} + \mathbf{P}^2 \mathbf{T} + \mathbf{P}^3.$$

But, the relation of arcs e and f of the nonzero (e, f) -array of $({}^T \mathbf{U})^3$ are divided into the eight cases in Figure 1. In fact, the cases I, II, III, IV, V, VI, VII and VIII correspond to the matrices \mathbf{T}^3 , $\mathbf{T}^2 \mathbf{P}$, \mathbf{TPT} , \mathbf{PT}^2 , \mathbf{TP}^2 , $\mathbf{P}^2 \mathbf{T}$, \mathbf{PTP} and \mathbf{P}^3 , respectively. In the case I, an (e, f) -path has no backtracking. For the cases II, III and IV, an (e, f) -path has exactly one backtracking. For the cases V, VI and VII, an (e, f) -path has exactly two backtrackings. In the case VIII, an (e, f) -path has exactly three backtrackings. All nonzero elements of $({}^T \mathbf{U})^3$ corresponding to cases II, III, IV and VIII are negative. Furthermore, all nonzero elements of $({}^T \mathbf{U})^3$ corresponding to cases I, V, VI and VII are positive. Thus, four matrices $\mathbf{T}^2 \mathbf{P}$, \mathbf{TPT} , \mathbf{PT}^2 and \mathbf{P}^3 are excluded. Furthermore, all positive elements of $({}^T \mathbf{U})^3$ and $\mathbf{T}^3 + \mathbf{TP}^2 + \mathbf{P}^2 \mathbf{T} + \mathbf{PTP}$ are in the same place.

Therefore,

$$\begin{aligned} ({}^T \mathbf{U}^3)^+ &= (\mathbf{T}^3 + \mathbf{TP}^2 + \mathbf{P}^2 \mathbf{T} + \mathbf{PTP})^+ \\ &= (\mathbf{T}^3 + \mathbf{T} + \mathbf{T} + \mathbf{PTP})^+ \\ &= (\mathbf{T}^3 + \mathbf{T} + \mathbf{PTP})^+. \end{aligned}$$

Since $g(G) > 4$, nonzero element of \mathbf{T}^3 and \mathbf{T} are not overlapped. If a nonzero (e, f) -arrays of \mathbf{T}^3 and \mathbf{PTP} are overlapped, then there exists an essential cycle of length four from e to f in G , contradiction to $g(G) > 4$. Furthermore, if a nonzero (e, f) -arrays of \mathbf{T} and \mathbf{PTP} are overlapped, then $f = e^{-1}$, and so the (e, f) -array is zero. Thus, nonzero elements of three matrices \mathbf{T}^3 , \mathbf{T} and \mathbf{PTP} are not overlapped.

But, all nonzero elements of two matrices \mathbf{T} and \mathbf{PTP} are 1. In the case of $g(G) > 4$, then all nonzero elements of the matrix \mathbf{T}^3 are 1. If an (e, f) -array of \mathbf{T}^3 is not less than 2, then there exist two distinct (e, f) -paths $P = (e, g, h, f)$ and $Q = (e, g_1, h_1, f)$ in G . Then the cycle $(g, h, h_1^{-1}, g_1^{-1})$ is an essential cycle of length four in G . This contradicts to the condition $g(G) > 4$.

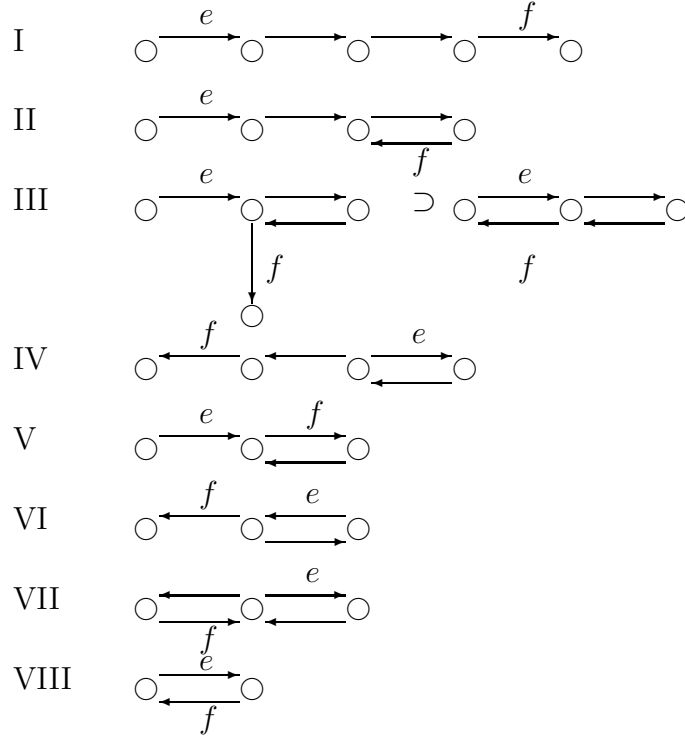


Figure 1 The nonzero (e, f) -array of $({}^T\mathbf{U})^3$.

Therefore, it follows that

$$(\mathbf{U}^3)^+ = ({}^T\mathbf{T})^3 + {}^T\mathbf{T} + \mathbf{P}^T\mathbf{T}\mathbf{P}.$$

Since ${}^T\mathbf{T} = {}^T\mathbf{B} - \mathbf{P} = \mathbf{U}^+$, we have

$$(\mathbf{U}^3)^+ = (\mathbf{U}^+)^3 + \mathbf{U}^+ + \mathbf{P}\mathbf{U}^+\mathbf{P}.$$

But, by Proposition 7.1,

$$\begin{aligned}\mathbf{P}\mathbf{U}^+\mathbf{P} &= \mathbf{P}({}^T\mathbf{D}_t\mathbf{D}_h - \mathbf{P})\mathbf{P} \\ &= \mathbf{P}^T\mathbf{D}_t\mathbf{D}_h\mathbf{P} - \mathbf{P}^3 \\ &= {}^T\mathbf{D}_h\mathbf{D}_t - \mathbf{P} = {}^T\mathbf{U}^+.\end{aligned}$$

Hence,

$$(\mathbf{U}^3)^+ = (\mathbf{U}^+)^3 + \mathbf{U}^+ + {}^T\mathbf{U}^+.$$

Thus, the following result follows

THEOREM 7.2 *Let G be a connected k -regular graph. Suppose that $k > 2$ and $g(G) > 4$. The positive support $(\mathbf{U}^3)^+$ is of the form*

$$(\mathbf{U}^3)^+ = (\mathbf{U}^+)^3 + \mathbf{U}^+ + {}^T\mathbf{U}^+.$$

Emms et al. [3] determined a necessary and sufficient condition for any array of $(\mathbf{U}^3)^+$ of a strongly regular graph to be equal to 1, and proposed the following conjecture:

CONJECTURE 7.3 (EMMS, HANCOCK, SEVERINI AND WILSON [3]) *Let G and H be strongly regular graphs with the same set of parameters. Then $G \cong H$ if and only if $\text{Spec}((\mathbf{U}(G)^3)^+) = \text{Spec}((\mathbf{U}(H)^3)^+)$.*

If we apply the linear algebraic technique of Godsil and Guo [7] to $(\mathbf{U}^3)^+$, and approach the characteristic polynomial of $(\mathbf{U}^3)^+$, then it might be likely to be able to determine the spectra of $(\mathbf{U}^3)^+$. Related to this conjecture, to find an explicit formula for the characteristic polynomial of the positive support $(\mathbf{U}^n)^+$ for any n would be one of the interesting future problems.

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